Superconducting Pair Fluctuations in $YBa_2Cu_3O_7$

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We report two complementary experiments that probe the magnetic field and temperature effects of superconducting pair fluctuations in $YBa_2Cu_3O_7$: (1) measurement of the Pauli spin susceptibility[1] and (2) measurement of the ^{63}Cu spin-lattice relaxation rate ($1/T_1$).[2] We compare our data with a theory[3] of superconducting fluctuations appropriate for a weak-coupling, quasi-2D, d-wave superconductor. The theory takes exactly into account dynamical fluctuations and includes a sum over all Landau levels to extend the range of validity to high fields and temperatures.

In Figure 1 we show ^{17}O NMR spin shifts that are proportional to the Pauli spin susceptibility, from 2.1 T to 24 T. The temperature dependence can be accounted for by superconducting pair fluctuations that result in a smooth crossover from the normal to the vortex liquid state. A detailed comparison with the theory at 8.4 T accurately reproduces the data down to 85 K.

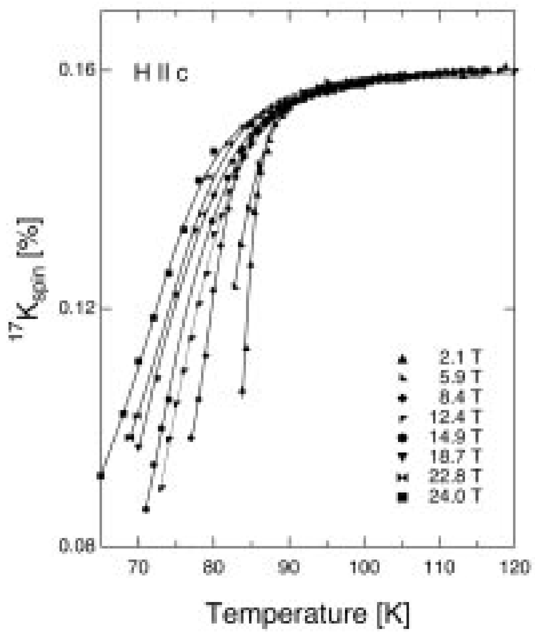

Figure 1. ^{17}O NMR shifts, proportional to Pauli spin susceptibility, in $YBa_2Cu_3O_7$. Lines are guides to the eye.

In Figure 2 we show the ^{63}Cu spin-lattice relaxation rates, $1/T_1T$ from 2.1 T to 27.3 T. For temperatures below 120 K, the spin-lattice rate increases with increasing magnetic field. We account for this increase quantitatively as the suppression of

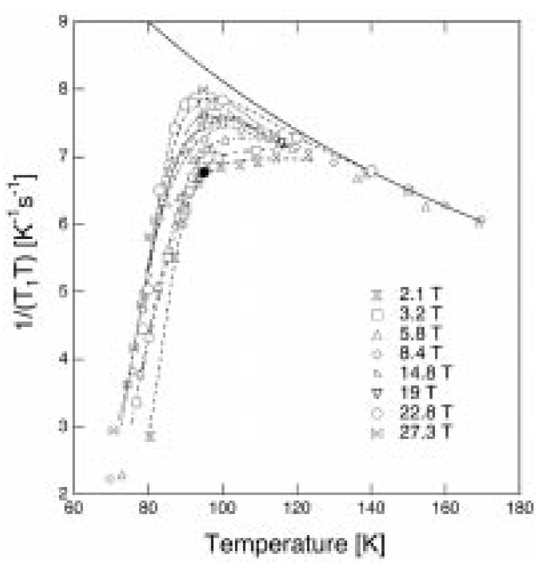

Figure 2. ^{63}Cu spin-lattice relaxation in $YBa_2Cu_3O_7$. Lines are guides to the eye. The data point at 95 K (●) is taken from Ref. 4, as discussed in the text.

negative contributions to the rate originating from density-of-states superconducting fluctuations with d-wave symmetry. Fluctuation contributions with s-wave symmetry would decrease the rate with increasing magnetic field in contrast with our observations. For comparison we also include a measurement by Gorny, *et al*.[4] Their lower result, shown as a solid circle and field independent for 0, 8.8, and 14.8 T, can be attributed to underdoping of their $YBCO_{7-\delta}$ sample.

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Transport Properties of the Ground State of $La_{2-x}Sr_xCuO_4$ High Temperature Superconductor

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$La_{2-x}Sr_xCuO_4$ (LSCO) is a high temperature superconductor with a transition temperature, T_c, as high as 40 K. While there is still no consensus on the origin of high temperature superconductivity, it is generally believed that the key to understanding can be likely found in the anomalous properties of the normal (non-superconducting) state of high T_c superconductors.[1] Although the T_c in LSCO can be as high as 40 K, one can suppress the superconductivity with 60 T magnetic field to study the normal state properties. When intense magnetic fields suppress the superconducting phase of the high T_c cuprates, insulating behavior is revealed in the underdoped regime for both in-plane (ρ_{ab}) and c-axis (ρ_c) resistivities. In LSCO, this low temperature insulating behavior ($d\rho/dT < 0$) has been observed to extend throughout the underdoped regime (i.e. for all $x < 0.16$).[2] The low temperature behavior of both ρ_{ab} and ρ_c in this regime is best described as a logarithmic dependence of the resistivity on temperature.[3] We measured transport properties of single crystal samples of $La_{1.92}Sr_{0.08}CuO_4$ for both in-plane and c-axis orientations.[4]

We developed the experimental setup for transport measurements in the 60 T Long Pulse magnet, which allows determining the absolute resistance with resolution of better then 200 μΩ. We investigated the extent of the logarithmic divergence of the resistivity in the low temperature limit, for transport within the Cu-O layers and perpendicular to the layers in this quasi two-dimensional compound. The insulating divergence of resistivity has been observed to temperatures as low as 350 mK, which extends previously reported temperature ranges by a factor of 2. We encountered some problems with build-up of

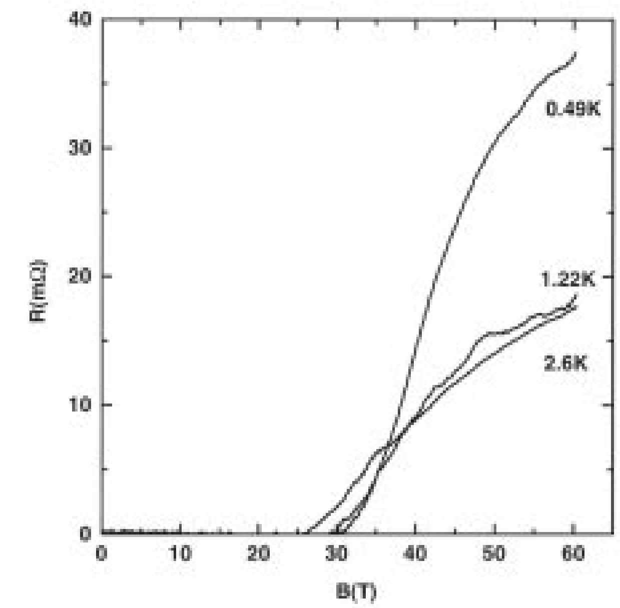

Figure 1. In-plane resistance of the $La_{1.92}Sr_{0.08}CuO_4$ sample vs. magnetic field. Superconductivity in the sample is suppressed above ~35 T. Normal state resistance increases dramatically as temperature decreases.

temperature gradients for measurements performed in liquid He^3, which needs to be straightened up for the future experiments.

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4. The logarithmic divergence of resistivity has been best established for the samples with Sr doping level x ~ 0.08.

Diagonalization in Reduced Hilbert Spaces Using a Systematically Improved Basis: Application to Spin Dynamics in Lightly Doped Ladders

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A method is proposed to improve the accuracy of approximate techniques for strongly correlated electrons that use reduced Hilbert spaces.[1] As a first step, the method involves a change of basis that incorporates exactly part of the short distance interactions. The Hamiltonian is rewritten in new variables that better represent the physics of the problem under study. A Hilbert space expansion performed in the new basis follows. The method is successfully tested using both the Heisenberg model, and the t-J model with holes on 2-leg ladders and chains, including estimations for ground state energies, static correlations, and spectra of excited states. An important feature of this technique is its ability to calculate dynamical responses on clusters larger than those that can be studied using Exact Diagonalization. The method is applied to the analysis of the dynamical spin structure factor S(q, ω) on clusters with 2 x 16 sites and 0 and 2 holes. Our results confirm previous studies (Troyer, M., *et al.*, Phys. Rev. B, 53, 251 (1996)), which suggested that the state of the lowest energy in the spin-1 2-holes subspace corresponds to the bound state of a hole pair and a spin-triplet. Implications of this result for neutron scattering experiments both on ladders and planes are discussed.

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Phase Fluctuations and the Pseudogap Phenomenon in the Underdoped Cuprate Superconductors

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One of the more intriguing properties of the cuprate superconductors is the existence of a "pseudogap" regime in the normal phase, which develops when these materials are underdoped and at temperatures below a characteristic temperature T^*. Recent angle-resolved photoemission (ARP ES) and scanning tunneling spectroscopy (STS) measurements on $Bi_2Sr_2CaCu_2O_{8+\delta}$ show that there is a gap in the single-particle excitation spectrum even though the sample is normal and the superfluid density is zero; the pseudogap appears to evolve smoothly from the superconducting gap. More significantly, the ARPES results show that the pseudogap in the normal phase possesses the same $d_{x^2-x^2}$ symmetry as the superconducting gap; the node along the (π/2,π/2) direction in the superconducting phase evolves into an extended gapless region with increasing temperature in the pseudogap regime, while the gap maximum in the (π, 0) direction has only a very weak temperature dependence. Taken collectively, these results indicate that the pseudogap in the normal phase is a remnant of the quasiparticle gap in the superconducting phase.

The theoretical challenge in understanding the pseudogap regime is then to reconcile the existence of a quasiparticle gap with the absence of superconducting order. One resolution, proposed by Emery and Kivelson, is that local superconducting order exists, but long range phase coherence, the hallmark of the superconducting state, is destroyed due to strong phase fluctuations. The phase fluctuations in the cuprates are expected to be larger than in conventional superconductors due to the low superfluid density (a characteristic of doped Mott insulators).

We adopt this point of view in our work,[1] and ask what effect these phase fluctuations would have on the single particle properties which are measured in either ARPES or STS experiments. In our model the fluctuating phase induces a fluctuating Doppler shift in the spectrum of the quasiparticles. The properties of the transverse phase, or vortex, fluctuations change dramatically as one approaches the superconducting transition, which in our two dimensional model is a Kosterlitz-Thouless vortex-pair unbinding transition. In passing through this transition there is a significant broadening of the quasiparticle spectral function and a distinct pseudogap feature, similar to what is observed in the ARPES experiments. These results are currently being extended to include the effects of amplitude fluctuations; we hope in the future to be able to calculate transport properties within this framework.

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Physics of High Temperature Superconductors

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The physics of high temperature superconductors is incompletely understood, and remains one of the major unsolved problems in condensed matter physics. We have attempted to contribute to the solution of this problem (A) by successfully predicting new superconductors,[1,3,4,6] and (B) by proposing a new theory of homologues of $Nd_{2-z}Ce_zCuO_4$ and related high temperature superconductors. In the case of $Nd_{2-z}Ce_zCuO_4$, these materials are thought to be *n*-type superconductors, but we argue that they must be *p*-type. If we are correct, bipolar superconducting electronics with the conventional high temperature superconductors will be impossible.

A. *New Superconductors*: We have successfully predicted that $PrBa_2Cu_3O_7$, long thought to be an insulator of choice, is in fact a ≈ 90 K superconductor, if it is grown defect free.[6] We have shown that experimentally this is indeed the case. A by-product of this demonstration is strong evidence that the primary superconductivity does not originate in cuprate planes (as once widely believed), but that the origin of superconductivity is in the charge-reservoir regions of the various crystal structures.[2,5] We have similarly shown that $Gd_{2-z}Ce_zSr_2Cu_2TiO_x$ (with $x \approx 10$) and $Pr_{2-z}Ce_zSr_2Cu_2NbO_{10}$, both once thought to *not* superconduct, are actually robust superconductors when defect-free.[1,4]

These are the only three high temperature superconductors to date (to our knowledge) that have been *predicted to superconduct* before they were shown experimentally to do so, and give us optimism about our fourth prediction: that $Am_{2-z}Ce_zCuO_4$ will also superconduct.

B. *Homologues of $Nd_{2-z}Ce_zCuO_4$ and Related Superconductors*: Arguments are presented that the $Nd_{2-z}Ce_zCuO_4$ superconducting homologues, the so-called “electron-doped” or “*n*-type” superconductors, are actually doped *p*-type by (Ce, $O_{interstitial}$) pairs, rather than *n*-type by isolated Ce (as widely believed). This implies that bipolar high temperature superconducting electronics are impossible, because all high temperature superconductors are *p*-type. The compatibility of various rare earth ions (R) with, or without, superconductivity in the compounds $RBa_2Cu_3O_7$, $RBa_2Cu_4O_8$, $RBa_2Cu_2NbO_8$, $R_{2-z}Ce_zCuO_4$, and $R_{2-z}Ce_zSr_2Cu_2NbO_{10}$, and their homologues, are predicted, and defects that play central roles in their

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superconductivity (or not) are described. The role of Th-doping *versus* Ce-doping is discussed with emphasis on those materials for which only one of the two dopants should produce high temperature superconductivity.

The importance of the superconductivity residing primarily in the charge-reservoir layers (and not in the cuprate planes) is discussed, producing a new picture of high temperature superconductivity that is compatible with many data.[7,8,9]

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Hole-Pairs in a Spin Liquid: Influence of Electrostatic Hole-Hole Repulsion

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The stability of the bound state of holes in the t-J model, including short-range Coulomb interactions, was analyzed using computational techniques on ladder geometries with up to 2 x 30 sites. For a nearest-neighbors (NN) hole-hole repulsion, the two-hole bound state was shown to be surprisingly robust, and it breaks only when the repulsion is several times the exchange J. It was also observed that at ≈ 10% hole doping the pairs break only for a NN repulsion as large as V ≈ 4J. Our results support electronic hole-pairing mechanisms on ladders based on holes moving in spin-liquid backgrounds. Implications for similar scenarios in two dimensions were also investigated. The need for better estimations of the range and strength of the Coulomb interaction in copper-oxides was one of our conclusions.

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Problem of Quantum Oscillations in Superconducting Mixed State

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In normal metals de Haas van Alphen (dHvA) oscillations measure directly the Fermi surface shape and size. While the dHvA effect in the normal phase arises from electron levels quantized in the field, B, passing through the chemical potential μ, the excitations of a superconductor are a mixture of particles and holes and are gapped, with the chemical potential seated at the center of the gap. In the limit $Hc_1 << B << Hc_2$ low energy excitations persist only at the centers of the vortex line. The vortex cores occupy only a small fraction of the volume and may be neglected. In the above limit B would be nearly uniform in space.

We have studied the dHvA oscillations for this extreme limit being motivated by the experimental observations of the dHvA oscillations in the superconducting state for magnetic fields as low as $0.2Hc_2$. The theoretical expectations are that the dHvA signal is to rapidly decay with the field decrease, in accordance with the fact that excitations levels are now gapped and spread out symmetrically about μ. Therefore, the dHvA effect in superconducting state at $B << Hc_2$ occurs for a different reason.

Since the Larmour radius of the orbits is large, one can use the WKB approximation. This was accomplished in[1] by writing the system of Gor'kov equations in coordinates attached to an electron moving along the cyclotron orbit. In[1] it was shown, in addition, that even a superconducting order parameter with zeroes in the gap (d-wave pairing) does not restore the mechanism of crossing the chemical potential by excitations, levels, which is the cause of the dHvA effect in the normal state.

Recently we found a new mechanism[2-5] for the dHvA oscillations in a superconductor based on two types of states that occur in the presence of B. These two types of states are localized and delocalized states depending on the excitations energy. One mechanism for localization and formation of an energy threshold arises from the Doppler shift: $E(p)\rightarrow E(p)=E(p)+p\cdot v_s(r)$ where the superfluid velocity, is due to supercurrents flowing around the vortices. The electron sees a random potential as it moves around its classical trajectory, in this case, in the magnetic field. Below a threshold energy, $|\Delta|+|p\cdot v_s(r)|max$, the supercurrents cause localization of states. The second effect is the gap anisotropy. In this case only states whose energy lies above the maximum gap can be extended states.

One finds that the variation of magnetization with the change of the magnetic field results in many harmonics in the dHvA signal. The large result for a particular potential along the Larmour orbit is considerably reduced by averaging over orbits centered at any point in the vortex lattice. The averaging process results on an estimate for the effective Dingle temperature of $\Delta(\xi_o/d)$.

Thus instead of Dingle temperature being of the order $1/\tau\sim\Delta$, as it is commonly expected for an s-wave superconductor, one finds this temperature reduced by the factor $(\xi_o/d)<<1$.

Thus excitations in a superconductor at $B<<Hc_2$ occur in two types, localized and delocalized ones. Levels crossing the threshold separating these two types of states lead to the dHvA oscillations in superconducting state at $B<<Hc_2$. We believe that this mechanism may account for the dHvA oscillations observed at $B\sim 0.2Hc_2$.

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Magnetic Field Independence of the Spin Gap in $YBa_2Cu_3O_{7-\delta}$

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A dominant feature of optimally and underdoped cuprates is the appearance of a pseudogap in the normal state excitation spectrum. The high magnetic field behavior of the pseudogap provides additional experimental characterization of the pseudogap that is crucial for differentiating between various pictures. We report very high accuracy measurements of the magnetic field dependence of the ^{63}Cu spin lattice relaxation rate in near optimally doped $YBa_2Cu_3O_{7-\delta}$. Our measurements demonstrate, in sharp contrast with previous work, that there is no magnetic field dependence to $^{63}(T_1T)^{-1}$ in $YBa_2Cu_3O_{7-\delta}$ to an uncertainty of 2 K up to 14.8 T, which suppresses

T_c by 8 K. The ^{63}Cu NMR spin lattice relaxation rate reveals the spin part of pseudogap behavior. In underdoped $YBa_2Cu_3O_{6.6}$, $^{63}(T_1T)^{-1}$ exhibits a broad maximum in the vicinity of room temperature and then decreases as T approaches T_c from above. In optimally doped $YBa_2Cu_3O_{7-\delta}$ (Figure 1) the maximum occurs at ª 110 K, and commences a quite steep descent as T is lowered toward T_c = 93. The steepness of the downturn of $^{63}(T_1T)^{-1}$ enables a sensitive measurement of the field dependence.

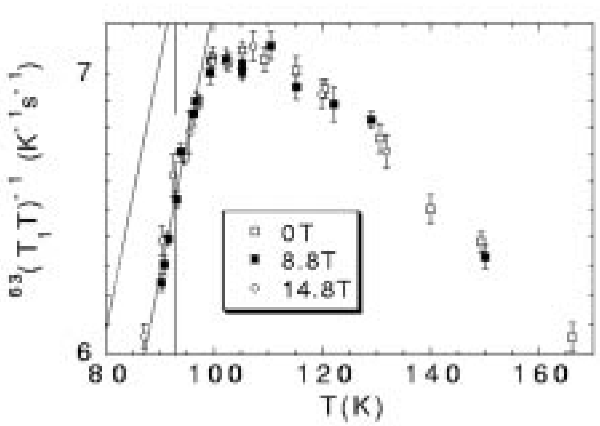

Figure 1. $^{63}(T_1T)^{-1}$ vs. T for magnetic fields (applied along the crystal c axis) of 0, 8.8, and 14.8 T.

This result has three important ramifications. Although the magnetic fields we apply shift T_c down by as much as 8 K, the onset of pseudogap effects does not shift down in temperature. Hence the pseudogap is unrelated to superconducting fluctuations, even in near-optimally doped samples where the gap behavior appears just above T_c. The onset of the pseudogap is very rapid, clearly demonstrating that its magnitude is temperature dependent, opening very rapidly near 110 K. The absence of any field effect indicates a relatively large energy scale for the gap mechanism. If dynamical pairing correlations or pre-formed pairs are involved, the length scales must be very short. These results would appear to call for relatively large energy and short length scales in a scenario involving dynamical pairing correlations or pre-formed pairs.

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Quasiparticles in *d*-Wave Superconductors

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Quasiparticle contribution to thermodynamics and transport in vortex state. A theory of the vortex state in clean and disordered *d*-wave superconductors was constructed with an eye toward understanding recent experiments on cuprate and heavy fermion superconductors. The simple underlying picture is that, in contrast to classic *s*-wave systems, the few bound states in vortex cores are irrelevant, and the principal contribution arises from the extended states located in momentum space near the d-wave nodes. In such a case, there is a range of fields and temperatures, which we argue to be surprisingly large in the cuprates, where the principal contribution to the magnetic field dependence of both thermal and transport properties arises from the changes in quasiparticle occupation number due to the Doppler shift of the quasiparticle energy in the vortex superflow field.

In the past year, we calculated thermal transport properties at low temperatures and field scales small compared to H_{c2}. The remarkable result of such a theory is that the thermal conductivity increases with field as roughly H log H, in dramatic contrast to traditional theories of vortex scattering, which predict a decrease with field. These predictions, including dependence on disorder, were dramatically verified recently by experimentalists at McGill/Toronto and Orsay. We also calculated thermodynamic and transport properties for field parallel to the CuO_2 layers, a somewhat more complicated problem, and predicted 4-fold oscillations of the density of states (DOS) as a function of angle of the magnetic field relative to the crystal axes, different power laws and magnetic scaling functions for the DOS according to whether the field was aligned with the gap nodes or not.

Nonlocal and nonlinear electrodynamics in a d-wave superconductor. (With P. Woelfle, Univ. of Karlsruhe).

In the case of a weak field, the current response of the *d*-wave superconductor at low temperatures has long been treated in a local approximation. Recently, Kosztin and Leggett (KL) showed that the nonlocal response of the condensate cannot be neglected at the lowest temperatures despite the fact that the in-plane coherence length ξ_0 is nominally two orders of magnitude smaller than the penetration depth λ_0 since the effective coherence length for the quasiparticles is v_F/Δ_0, which diverges along the nodal directions. Although in the cuprates this is important only at extremely low temperatures the nonlocal energy E_{nonloc} can compete with other energies, like the impurity scale γ or the nonlinear field scale E_{nonlin} at easily accessible laboratory fields, leading to new physics. We have begun an investigation of the competition of these effects in a *d*-wave superconductor, and shown, as a first step, that nonlocal electrodynamics are probably responsible for the failure to observe the nonlinear Meissner effect despite considerable experimental effort.

Search for Reentrant Superconductivity in Sr_2RuO_4

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The layered oxide compound Sr_2RuO_4 is considered to be a superconductor[1] with triplet pairing, based upon the nonmagnetic impurity concentration dependence of T_c, NMR-Knight shift, μSR, specific heat in the magnetic field and H_{c2} anisotropy. In this case, the magnetic energy to be stored in spin system does not work to destroy the superconductivity provided that the orbital magnetization is suppressed. Lebed and Yamaji[2] predicted that the superconductivity of Sr_2RuO_4 suppressed by the magnetic field as low as 2 T can be restored in the high magnetic field exceeding 35 T to 50 T, provided that the superconductivity is of really triplet nature. For the experimental observation, it is essential to apply the magnetic field along the conducting plane with the accuracy less than 0.01° so that the perpendicular component does not exceed H_{c1} and does not induce the orbital effect.

We had carried out the preliminary experiment at Kyoto with use of a 17 T magnet keeping a sample at 0.1 K to establish the experimental procedure in particular with respect to the alignment of the field orientation with the accuracy of less than 0.01°. It was also important to characterize the samples, since the superconducting behavior depends on the purity. We prepared samples with T_c of 1.41 K. The in-plane and out-of-plane resistances of measured samples at 1.5 K were 34 μohm and 2.0 mohm, respectively. The experiment at NHMFL was carried out with the resistive magnet of 30 T with 32 mm bore. The sample was cooled to 0.5 K in He-3 cryostat and rotated quasi-continuously with a sample rotator. Although the backlash caused a time-consuming process, the angle was scanned to detect the change on appearance of the superconductivity when the width of the angle is in the order of 0.01°. We tried to detect the change in the in-plane resistance with the current direction almost parallel to the field direction to avoid the dissipation due to the vortex motion. The procedure was as follows: first determine the direction by monitoring the resistance minimum appearing sharply near 1.6 T which is close to H_{c2}, increase the field to 30 T and then make angle sweep to find the resistive decrease due to superconductivity. The last procedure is necessary since the change in the field alignment can be disturbed during the field increase. We could carry out the first procedure successfully, however, with increase of the field, we met the problem of the increase in noise that grew so as to exceed the level of the signal at 30 T. As a most probable origin of the noise, we point out the effect of slight oscillation of wiring to feed the measurement current in the high magnetic field. We also carried out the measurement for the out-of-plane resistance. In this case the noise was not fatal to detect the resistance decrease due to superconductivity if it appeared, but we cannot rule out the possibility that the dissipation due to the vortex motion masked the resistive decrease. By exploring a way to suppress the effect of the noise, we are willing to challenge the subject.

We should acknowledge M. Whitton and J. Qualls for their invaluable help and S. Hannahs and B. Brandt for their support and guidance. The work was supported also by Japan Science and Technology Corporation.

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Point Disorder Induced Transition in the Mixed State of $YBa_2Cu_3O_7$

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The influence of quenched random pinning on the thermodynamic vortex phases has been a subject of intense scientific interest. In high temperature superconductors, point disorder is responsible for the destruction of the melting transition[1] and for the creation of the high magnetic field glassy phase.[2] In general, it is supposed that the amount of disorder needed to destroy the vortex solid-to-liquid first order melting transition is comparable to the one needed to disorder the vortex lattice into a glass. This produces a phase diagram where the lattice-glass coexistence line meets the lattice-liquid line at the critical point.[3] Here we show that this situation is characteristic of dirty samples, and that in clean samples the lattice-glass line terminates at the melting line well below the critical point.

We have performed transport measurements in a high quality, untwinned $YBa_2Cu_3O_7$ crystal, with the magnetic field parallel to the c-axis, in order to determine the magnetic field-temperature phase diagram. In Figure 1, we show the phase diagram before and after proton irradiation. The solid lines correspond to the sample before irradiation. The critical point indicates, and is evident from the data, that it does not coincide with the termination point of the lattice-glass transition line. After irradiation by protons to increase the density of point defects, the critical point moves down along the melting line approaching the lattice-glass line. As a consequence, the critical point will coincide with the termination point of the lattice-glass line for strong enough disorder. This indicates that in clean samples and for fields just below the critical point, it is possible to observe a first order melting transition between a glassy-vortex phase and a liquid state.

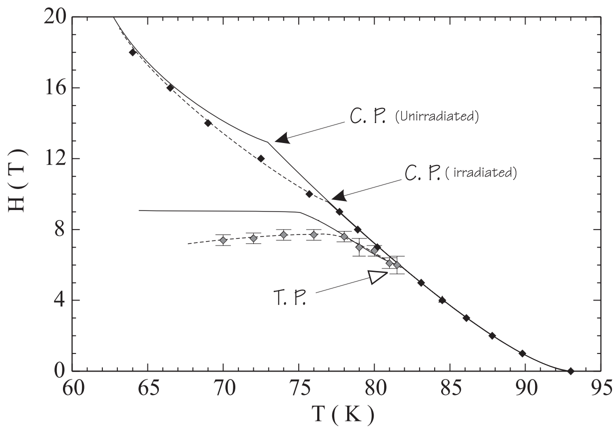

Figure 1. (H-T) phase diagram of an untwinned $YBa_2Cu_3O_7$ crystal before and after proton irradiation.

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Dynamic and Static Properties of Hole-Doped 4-Leg Ladders Using the Optimized Reduced Basis Approximation Method

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We used the Optimized Reduced Basis Approximation (ORBA) method[1] to calculate static and dynamic properties of the t-J model in 4-leg ladders. Our calculations include spin and charge correlations, as well as S(q,ω) and A(q,ω) (PES and IPES) on 4 x 8, 4 x 10, and 4 x 12 ladders at finite hole dopings. Several boundary conditions were used, and a wide range of doping was investigated. Specially for the 1 hole problem, we analyzed how the properties of the system varied with the ratio J/t, and compared the results with ARPES data for the undoped cuprates. Right now we are expanding the calculations to show that the ORBA method can also be applied to the t-t'-J model on 4 x N systems.

This work was supported by an NHMFL In-House Research Program grant.

Reference:

1 Dagotto, E., *et al*., Phys. Rev. B, 58, 12063 (1998).

Hole-Density Evolution of the One-Particle Spectral Function in Doped Ladders

NHMFL

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The spectral function A(q, ω) of doped t-J ladders was calculated on clusters with up to 2×20 sites at zero temperature applying a recently developed technique that uses up to 6×10^6 rung-basis states. Similarities with photoemission results for the 2D cuprates were observed, such as the existence of a gap at (π, 0) near half-filling (caused by hole pair formation), and flat bands in its vicinity. These features should be observable in ARPES experiments on ladders. The main result of our work is the nontrivial evolution of the spectral function from a narrow band at $x = 0$, to a quasi-noninteracting band at $x \geq 0.5$. It was also observed that the low energy peaks of clustered spectra acquire finite linewidths as their energies move away from the chemical potential.

This work was supported by an NHMFL In-House Research Program grant.

Phase Transition into Superconducting Mixed State and de Haas-van Alphen Effect

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The growing body of measurements demonstrates the presence of the de Haas-van Alphen effect in the mixed state of type-II superconductors. The theoretical description of this phenomenon is rather cumbersome, and as a result there is a vast amount of publications devoted to the subject. I performed the derivation of the Landau expansion of the free energy in the vicinity of the upper critical field, in powers of the square modulus, of the order parameter averaged over Abrikosov lattice. This problem has been treated earlier for 2-dimensional electron gas either numerically, or analytically, but out of the de Haas-van Alphen observation region, where the temperature exceeds the distance between the Landau levels.

I do it analytically for 3-dimensional isotropic BCS models under conditions of low temperature, and high enough purity that the de Haas-van Alphen effect in the normal state occurs. The calculations have been performed beyond the limits of quasiclassical approximation, with Landau quantization of the quasiparticle energy levels taken into consideration. The de Haas-van Alphen oscillations of the critical temperature, the order parameter's amplitude, and the magnetization in the mixed state are found. As in the normal metal case, the tiny oscillating corrections to the free energy are transformed into big summands, in a magnetic moment, as a result of the differentiation of very fast oscillating functions of the ratio of Fermi energy to the cyclotron frequency.

The work was performed from September to October 1998, during my stay at the NHMFL as a visiting scientist. The results were presented as a poster at the Conference on Physical Phenomena at High Magnetic Fields-III (24-27 October, Tallahassee) and will be published in the Proceedings of the Conference. The details of the calculations, as well as the discussion of the role of Pauli paramagnetic terms, and also the fluctuation effects near the transition, will be later submitted in Physical Review B.

Magnetoresistance of Hg-1223 Films

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We have measured the magnetoresistance (MR) in superconducting underdoped Hg-1223 films (T_c = 120 K) prepared by the sol-gel method on (100)-oriented $Y_{0.15}Z_{0.85}O_{1.93}$ single crystal substrates. The Hg-1223 crystallites in these films grow parallel to the substrate with the c-axis perpendicular to it.

Resistance vs. magnetic field in the range 0 T to 32 T was measured for isotherms: 4.2 K to 300 K. These measurements were performed for a current density of ≈ 10 amp/cm^2 flowing in the a-b plane of the Hg-1223 films. The MR was measured for I ⊥ H, and for I || H.

We observe:

a. High anisotropy of MR for I ⊥ H as compared to I || H.
b. Intermittent penetration of magnetic flux in the transition region from the superconducting to the normal state as demonstrated by the staircase response of MR.
c. Linear extrapolation of the normal state resistivity to zero state resistance for H = 32 T and for T → 0 K.
d. Negative MR for small field, H<2 T, when H ⊥ I, and for temperatures in the transition region. Positive MR for higher fields follows this trend.

Two Holes in a Locally Antiferromagnetic Background: The Role of Retardation and Coulomb Repulsion Effects

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The problem of two holes in the presence of strong antiferromagnetic fluctuations is revisited using computational techniques.[1] Two-dimensional clusters and 2-leg ladders are studied with the Lanczos and Truncated Lanczos algorithms. Ladders and square clusters of 32 sites are studied. The motivation of the paper is the recently discussed spatial distribution of holes in ladders, where the maximum probability for the hole to hole distance is obtained at $d = \sqrt{2}$ in units of the lattice spacing, a counter-intuitive result considering that the overall symmetry of the two-hole bound state is $d_{x^2-y^2}$. Here this effect is shown to appear in small ladder clusters that can be addressed exactly, and also in planes. The probability distribution of hole distances (d) was found to be broad with several distances contributing appreciably to the wave function. The existence of holes in the same sublattice is argued to be a consequence of non-negligible retardation effects in the t-J model. Effective models with instantaneous interactions nevertheless capture the essence of the hole pairing process in the presence of short-range antiferromagnetic fluctuations (especially regarding the symmetry properties of the condensate), similarly as the (non-retarded) BCS model contains the basic features of the more complicated electron-phonon problem in low temperature superconductors. The existence of strong spin singlets in the region, where the two hole bound state is located, is here confirmed, and a simple explanation for its origin in the case of planes is proposed using the Néel state as a background, complementing previous explanations based on a spin liquid undoped state. It is predicted that these strong singlets should appear regardless of the long distance properties of the spin system under consideration, as long as the bound state is $d_{x^2-y^2}$. In particular, it is shown that they are present in an Ising spin background. Finally, the influence of a short-range Coulombic repulsion is analyzed. Rough estimations suggest that at a distance of one lattice spacing this repulsion is larger than the exchange J. The hole distribution in the $d_{x^2-y^2}$ bound state is reanalyzed in the presence of such repulsion. Very short hole to hole distances lose their relevance in the presence of a realistic hole to hole interaction.

Reference:

1 Riera, J., *et al*., Phys. Rev. B, 57, 8609 (1998).

Magnetoresistance in Superconducting $Sm_{1.83}Ce_{0.17}CuO_{4-y}$

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We have performed measurements of magnetoresistance, R(T, H), in applied magnetic fields up to 18 T in granular samples of the electron-doped superconductor $Sm_{1.83}Ce_{0.17}CuO_{4-y}$. The samples were compacted under different pressures before sintering, i.e., 116, 147, and 245 MPa; and thereafter called S-116, S-147, and S-245, respectively.

The results of magnetization revealed superconductivity below $T_{ci} \approx 19$ K in all samples investigated. For samples S-116 and S-147, the R(T, H) curves were similar and showed an abrupt increase in the magnitude of R(T) below T_{ci}. Typical R(T) curves for the sample S-147 are shown in the Figure 1. The resistance excess, $\Delta R(T, H)$, exceeding the normal state resistance value, decreases with increasing H. It is not zero even in applied magnetic field as high as 17 T. We have also found that $\Delta R(T, H) \propto (T/T_{ci})^{-4}$ close to T_{ci}, in complete agreement with the predictions of the two-fluid theory.[1] For the

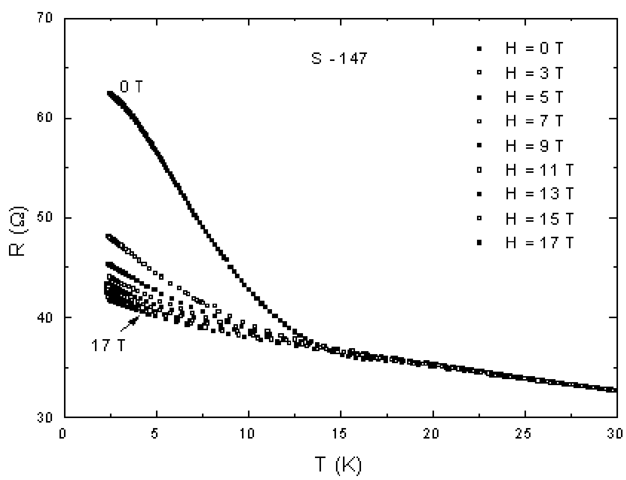

Figure 1. R(T) curves for the sample S-147 for 0 < H < 17 T.

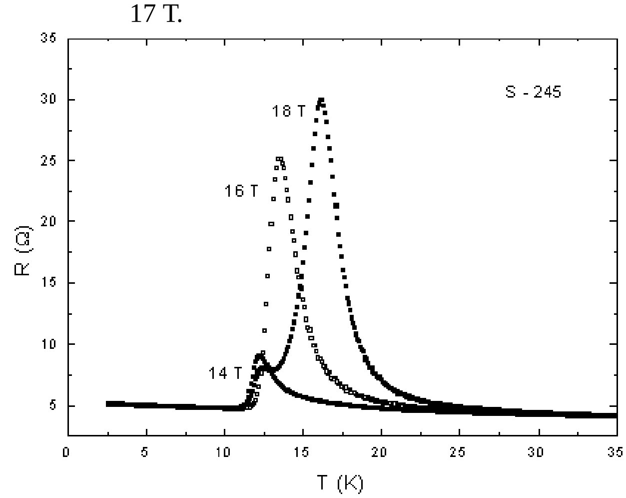

Figure 2. R(T) curves for the sample S -245 for H = 14, 16 and 18 T.

sample S-245, however, we have observed the appearance of a systematic peak in R(T,H) curves. The resistance maximum evolves with the magnetic field, revealing a giant magnetoresistance effect, as we can see in Figure 2. We have performed measurements of R(H), $0 < H < 18$ T, for several temperatures in the range 3 K < T < 50 K, and no hysteresis has been observed. We have found that these peaks are related to the melting of the Abrikosov vortex lattice.[2] This point is now being explored.

This work is supported by FAPESP under Grant No. 96/8416-4, the U.S.–Brazil Cooperative Research under Grant No. 910.101/97-3, and the Department of Energy (USA).

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Calorimetric Study of Flux-Lattice Melting in YBCO

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In the original discovery of flux-lattice melting in a detwinned single crystal of YBCO[1] at LBNL, our magnetic fields extended only to 9 T. Those experiments indicated that the latent heat of the first-order melting transition was decreasing and would probably vanish at a critical point at some higher magnetic field. An apparatus, using the same Differential Thermal Analysis (DTA) technique used at LBNL, was designed for use in the 20 T magnetic facility at the NHMFL-LANL, and was constructed at the University of California at Berkeley. This apparatus was to be used to extend the investigation of flux-lattice melting in YBCO to above 9 T.

In our first experiments at NHMFL, we calibrated the DTA platinum resistance thermometer in fields to 18 T. Attempts to measure the flux-lattice melting failed, however, because the Variable Temperature Insert (VTI), used with the 20 T Cryostat, was unable to maintain the background “bath” temperature sufficiently constant. (The flux-lattice melting in YBCO is detected as a very small part of the measured signal. Any small variation in the VTI temperature introduces noise to the differential signal being measured by a picovoltmeter that is comparable, or larger, than the effect to be observed.) The apparatus was subsequently altered to enable the DTA insert to be directly immersed in the helium bath of the cryostat at a stable 4.2 K.

Experiments done on the second visit to NHMFL, using the modified DTA insert, produced excellent data that showed clearly the vanishing of the first-order melting transition at a critical field of 10.5 T. Above 10.5 T there remained a “step” in the specific heat, but no evidence of a latent heat. The critical point at 10.5 T is believed to be a tricritical point. In experiments planned for 1999, we will make magnetic field scans at fixed temperatures in an attempt to locate the boundary between the two regions, i.e., the regions with and without a latent heat.

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1 Schilling, A., *et al.*, Nature, 382, 791 (1996).

Magnetoresistance of $TmNi_2B_2C$

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Lacerda, A.H., NHMFL/LANL
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We have measured the transverse magneto-resistance of $TmNi_2B_2C$ from about 2 K to

40 K with the field aligned along the [001] and [100] axes. $TmNi_2B_2C$ exhibits a superconducting transition near 11 K, and a magnetic transition near 1.5 K.[1] The magnetic state of $TmNi_2B_2C$ has been characterized as resulting from a transversely polarized spin density wave with moments aligned along the c-axis.[2]

With H // [100] we find a monotonic, positive magnetoresistance that reaches about 12% at 18 T and 2 K. With H // [001] we find a negative magnetoresistance in low fields followed by a positive magnetoresistance to the highest fields measured. A broad minimum in the magnetoresistance separates the two regimes. We attribute this behavior to the quenching of magnetic scattering associated with antiferromagnetic spin fluctuations.

This attribution, however, may be overly simplistic since we observe the field at which the minimum in the magnetoresistance occurs, Hmin, to increase with increasing temperature. We find that Hmin increases linearly from an extrapolated value of about 1 T at T=0, with a slope of about 0.6 T/K, to about 7 K after which the slope begins to decrease. The temperature dependence of Hmin is very small above about 30 K, where it reaches a value of about 9 T. One might expect such a temperature dependence to be associated with ferromagnetic spin fluctuations. Further work will address this intriguing possibility.

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Collective Excitations in High Temperature Superconductors

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Salkola, M.I., NHMFL

Collective low-lying excitations[1] in quasi-two-dimensional d-wave superconductors are explored. While the long-range Coulomb interaction shift longitudinal modes to high energy, spin wave excitations due to strong short-range interactions can propagate as damped collective modes within the superconducting gap. These excitations are suggested to be relevant to high temperature superconductivity, and may lead to distinctive signatures in the spectral density and neutron scattering data. Surprisingly, there is a range of momenta for which the spin fluctuations are sharp modes with no damping.

Reference:

1 Salkola, M.I., *et al.*, Phys. Rev. B, 58, 5944 (1998).

Collective Modes and Pseudogaps in HTS Materials

Schrieffer, J.R., NHMFL/FSU, Physics

The role of collective modes in determining the ARPES spectrum of Bi2212 is being studied in regard to the high energy broad maximum, at of order 100-150 meV, for emission in the (1,0) direction in contrast to the (1,1) direction. In the former case, the resonant scattering of a collective mode, presumably a spin fluctuation, by the photo hole leads to a broad peak without a quasi particle peak, as opposed to the (1,0) direction that is not resonant with this mode.

The observed pseudo gap in the ARPES spectrum of underdoped materials is presumably due to the existence of short range residual pairing order in the case that long range order is absent due to thermal fluctuations. At higher temperature, the short-range correlations are also broadened out and the material enters the peculiar metal regime.

Inhomogeneous States of Nonequilibrium Superconductors: Quasi Particle Bags and Anti-Phase Domain Walls

Schrieffer, J.R., NHMFL/FSU, Physics
Salkola, M.I., NHMFL

We studied the structure of excitations[1] in short coherence length superconductors. In contrast to low temperature superconductors in which the gap is uniform in space and depends only on the temperature, in HTS materials, one finds that a single quasi particle can lower the gap in its vacinity. The self-consistent solution of the Gor'kov equations show that two quasi particles are bound by the mutual sharing of a self-consistent bag. We have found that when forty quasi particles are present, the quasi particles form a ring with the order parameter charging sign across the domain wall inside to outside the ring. The spin density and spectral density of the quasi particles are localized on the domain walls. Thus, quasi particles interact strongly in short coherence material forming large structures. When all spins are spaced so that the quasi particles do not recombine. This may be studied by hole injection in a tunnel junction.

Reference:

1 Schrieffer, J.R., *et al.*, Phys. Rev. B, 57, 14433 (1998).

Numerical Study of Spin-Charge Separation in One Dimension

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Arrigoni, E., Univ. of Wurzburg, Germany, Physics
Hanke, W., Univ. of Wurzburg, Germany, Physics

Numerical studies of the existence of spin-charge separation were made in order to resolve the long standing issue of whether spin and charge excitations separate in two dimensional models of HTS materials. By studying spin and charge correlation functions it appears the spin and charge are not separated in two dimensions. A more direct measure of this separation is through the diagnostic operator that measures the product of the spin and charge densities as a function of spacing between the spin and charge operators. This method requires a larger size lattice to measure this quantity.

Unusual States of Inhomogeneous dsub(xsup$_2$ - ysup$_2$) + idsub$_{xy}$

Schrieffer, J.R., NHMFL/FSU, Physics
Salkola, M.I., NHMFL

Superconductors whose order parameter violates time-reversal symmetry and parity have unusual properties. If translation symmetry is also broken, the superconducting state spontaneously generates a current and a magnetic field. Some of the most striking consequences of the symmetry breaking are examined at boundaries, and in the presence of point-like impurities. We find that if the order parameter is a linear combination of d-wave xsup$_2$ -ysup$_2$ and imaginary xy, that states lie below the xy component of the gap due to self-consistent relaxation of the order parameter. These states generate a spontaneous current that flows in the presence of a wall or a defect. The magnitude of the magnetic field generated by these currents is 5 G.

Fermi Surface Study of the A15 Superconductor V_3Si

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Our ultimate aim in this study is to determine the Fermi surface in the A15 superconductor V_3Si and to explore the superconducting energy gap and its evolution on each part of the Fermi surface separately by observing de Haas-van Alphen (dHvA) oscillations in both normal and mixed states.

We carried out dHvA measurements up to 33 T and down to 0.6 K on single crystal samples of V_3Si. A phosphor bronze cantilever torquemeter similar to the one described in Ref. 1 was built and its small size enabled us to rotate a sample in a He^3 cryostat.

Figure 1 shows a dHvA oscillation trace measured along the direction 5 degrees from [100] in the (001) plane and its Fourier spectrum. The spectrum showing many close frequencies is a great contrast to those previously reported where only one or two frequencies were observed.[2,3] Angular dependence of dHvA frequencies in the (001) plane is shown in Figure 2. A gross trend is that most of the frequency branches move toward higher frequencies with tilting the field from [100], suggesting that they come from ellipsoidal Fermi surfaces elongated along [100] or arm-like structure running parallel to [100]. A previous band-structure calculation provides a few candidates of Fermi surface sheets that can account for the experimental results. However, to explain all the observed frequencies, it seems necessary to include domain formation due to the cubic-to-tetragonal structural transformation occurring slightly above T_c.

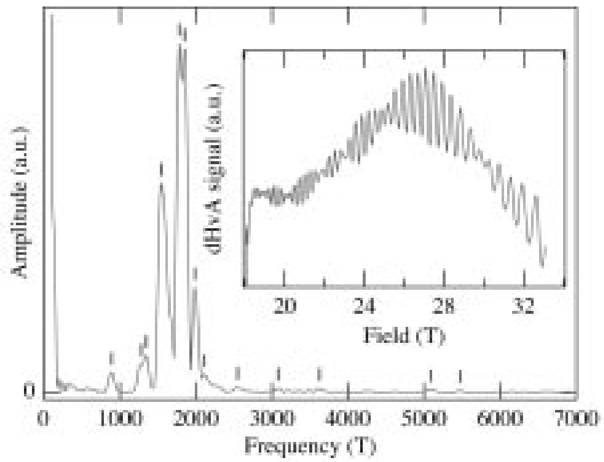

Figure 1. dHvA oscillation in V_3Si at 0.6 K for the field direction 5˚ from [100] (inset) and its Fourier

The efficiency of signal detection in the torque method decreases with decreasing field. In the present experiments, oscillating signals were already weak near H_{c2} even in the normal state and we could not see any dHvA oscillation in the mixed state. Therefore, we decided to employ the modulation technique to search for dHvA

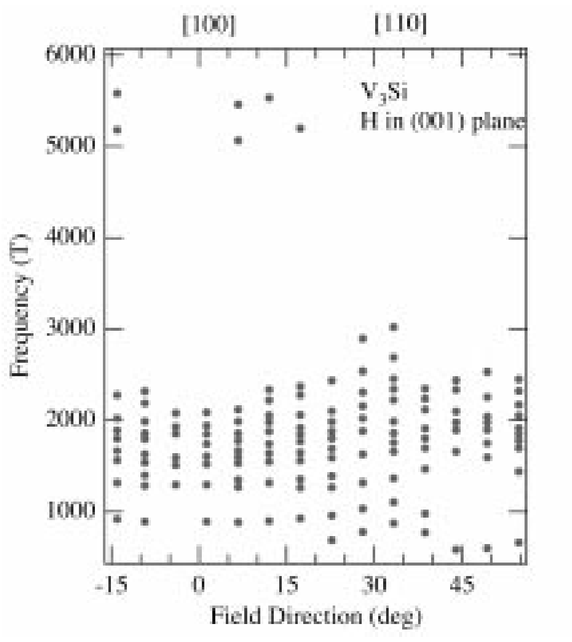

Figure 2. Angular dependence of dHvA oscillation frequencies in the (001) plane.

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oscillation in the mixed state. In the case of the field modulation technique, the detection efficiency can be enhanced to some extent at low fields by tuning the amplitude of the modulation field. In preliminary experiments done at Tsukuba Magnet Laboratory of NRIM, we have succeeded in observing dHvA oscillations in the mixed state. Modulation experiments will be continued both at NHMFL and NRIM.

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Responses to the High Magnetic Field of the Pseudogap and Superconductivity in High-T_c Cuprate

NHMFL

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It is now realized that the normal state of the underdoped high temperature superconductors cannot be understood within the framework of conventional theories. Of particular puzzling aspect is the appearance of the so-called "pseudogap" above the transition temperature T_c. This pseudogap is a phenomenon that the low energy spectral weight of the magnetic excitation is lost below a temperature that is much higher than T_c. In NMR measurements, both the temperature dependence of $1/T_1T$ and the Knight shift are anomalous. From the impurity effect on these anomalies, it was assigned that the temperature T^* below which $1/T_1T$ starts to decrease corresponds to the pseudogap temperature.[1] In $YBa_2Cu_4O_8$ (T_c = 80 K) which is a typical underdoped material, T^* = 160 K. Proposals for this phenomenon, include RVB singlet formation,[2] precursor of a spin density wave, and the superconducting fluctuations. Recent ARPES experiments that found the pseudogap evolves smoothly into the $d_{x^2-y^2}$ superconductivity have sparked wide interests about the origin of the pseudogap. In order to clarify the origin of the pseudogap, we have performed high magnetic field NMR studies in $YBa_2Cu_4O_8$. A field of 23.2 T parallel to the crystal c-axis reduces T_c by 20 K, or by 27% of its original value. This extends substantially the temperature range of the anomalous normal-state that was obscured by the occurrence of superconductivity at zero field. We have found that in contrast to such a large reduction of T_c, no change in the pseudogap was found. Also, in the temperature region where superconductivity was suppressed by the field, $1/T_1T$ extended its anomalous T-dependence seen at high temperatures. These results suggest that the pseudogap[3] is of magnetic origin, not due to the superconducting precursor such as preformed pairs or pairs without phase coherence, since one expects that the amplitude of such electron pairs will be suppressed by the field as happens below T_c.[4] The unconventional nature of the superconductivity in the high-T_c cuprates is also of great interest. In this study, we also examined the response of the superconductivity to magnetic field (H). From the measurement of $1/T_1$ and the spin Knight shift, we found a finite density of states at the Fermi level that is induced by the field. This finding indicates that the electronic states in the vortex core are ungapped and extend far outside the core. This is in contrast to the case of conventional superconductors, and is likely due to the anisotropic pairing symmetry of the d-wave superconductivity.

This study was done in collaboration with Y. Kitaoka, K. Asayama, and Y. Kodama.

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Anomalous SdH Oscillations in Organic Superconductor β”-$(BEDT\text{-}TTF)_2SF_5CH_2CF_2SO_3$

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Williams, J.M., Argonne National Laboratory

Magneto-transport measurements have been carried out in the dilution refrigerator with field up to 18 T in the organic superconductor β”-$(BEDT\text{-}TTF)_2SF_5CH_2CF_2SO_3$. Unlike other BEDT-TTF based organic superconductors, the Shubnikov de Hass (SdH) oscillations display a non-metallic temperature dependence of the background magnetoresistance.

Figure 1 is an overlay of SdH oscillation at various temperatures. The curve shifts upward with decreasing temperature. The background magnetoresistance can be reasonably fitted to a simple quadratic expression $R_0(H)=a+bH+cH^2$. With decreasing temperature, the oscillation amplitude increases in magnitude with a corresponding increase in the background resistance.

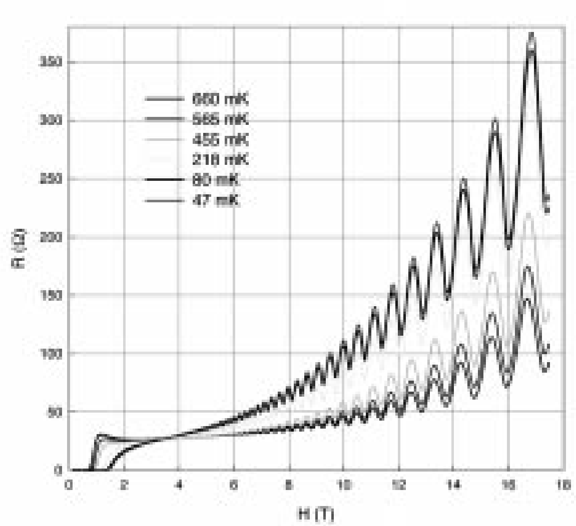

Figure 1. Field dependence of the interlayer resistance at different temperatures.

Shown in Figure 2 is a direct plot of the background magnetoresistance as a function of temperature at various fields from 9 T to 17 T with an increment of 1 T. The curves shift upwards with increasing field. At a fixed field, the resistance increases with decreasing temperature and tends to saturate at very low temperatures. At about 0.5 K, a stepwise increase in resistance is clear, especially at high fields. The relative increase in the magnetoresistance increases with increasing field.

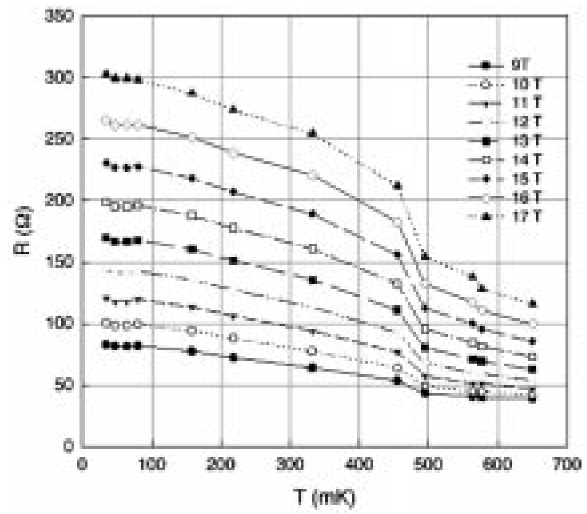

Figure 2. Temperature dependence of the background magnetoresistance at different fields.

The origin of the insulating behavior is not clear. One possibility is that a density wave is developed at low temperatures and high fields. In the 2D α-$(BEDT\text{-}TTF)_2MHg(SCN)_4$ with M = K, Rb, and Tl, a spin density wave is presumably observed at 8 to 10 K with a corresponding hump in resistivity.[1-2] In the quasi-1D system like $(TMTSF)_2X$ with X = PF_6, ClO_4, a field induced spin density wave has been observed.[3] The effect of magnetic field is to reduce the dimensionality of the electronic system. Magnetic field forces the electrons moving along open orbits to oscillate in the perpendicular direction of finite width. With increasing field, the width decreases and the charges are moving along an increasingly more 1D orbit, thus leading to the formation of a density wave. Band structure calculations predict the presence of open orbits in the studied compound. With increasing field, it is possible that partial nesting can rise from the open bands, resulting in a semiconducting like temperature dependence of the background magnetoresistance. In an ideal case the open bands contribute to the background magnetoresistance and the closed bands give rise to the SdH oscillation. The quadratic field dependence is generally consistent with the presence of open bands and this may also explain the normally large positive magnetoresistance observed in other 2D salts.[4] The absence of a thermally activated temperature dependence of the background resistance in the present compound suggests a partial nesting of the open bands, instead of a fully gaped state. Further work will be necessary to test the model.[4]

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Upper Critical Field Studies in Organic Superconductor κ-(BEDT-TTF)$_2$Cu(SCN)$_2$

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The layered organic molecular crystals κ-(BEDT-TTF)$_2$X where X is an anion are particularly interesting because they are strongly correlated electron systems with a number of similarities to the high-T_c cuprate superconductors including unconventional metallic properties and competition between antiferromagnetism and superconductivity. The availability of high quality single crystals combined with their lower superconducting transition temperature (T_c ~10 K) makes it possible to study experimentally the upper critical field in a steady magnetic field.

In this work, we report interlayer transport measurements carried out in the 30 T magnet on the organic superconductor κ-(BEDT-TTF)$_2$Cu(SCN)$_2$ studied as a function of temperature and angle between the sample and the field.[1]

For field parallel to the plane direction, the upper critical field extrapolated from the resistivity measurements exceeds substantially the simple BCS Pauli limit $H_p = 1.84\ k_B T_c$. Shown in Figure 1 is a plot of the H_{c2} as a function of temperature. Because of the relatively broad resistive transition in field, H_{c2} is not well defined. However, the critical field defined at the R = 1 Ω level (H_{c2}) as well as from extrapolation of superconducting and normal state field dependence (H_{c2}^*) shows similar quasi-linear temperature dependence. The zero temperature H_{c2} has a lower limit at about 30 T, compared to the H_p ~ 18 T.

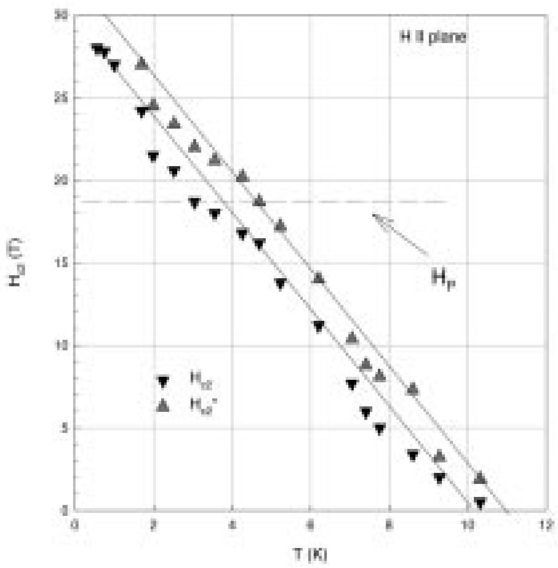

Figure 1. Temperature dependence of the upper critical fields.

The critical field thus defined is extremely sensitive to the field orientation with respect to the superconducting planes, especially near the field parallel to the plane geometry (θ = 90°). Shown in Figure 2 is a plot of H_{c2} defined at 1 Ω as a function of θ at T = 1.56 K. The two solid lines are fits to 3D and 2D models. The inset shows the expanded view near θ = 90°. Clearly, the 2D model fits the cusp-like feature of the data, while the 3D model is bell-shaped at this angle.[1]

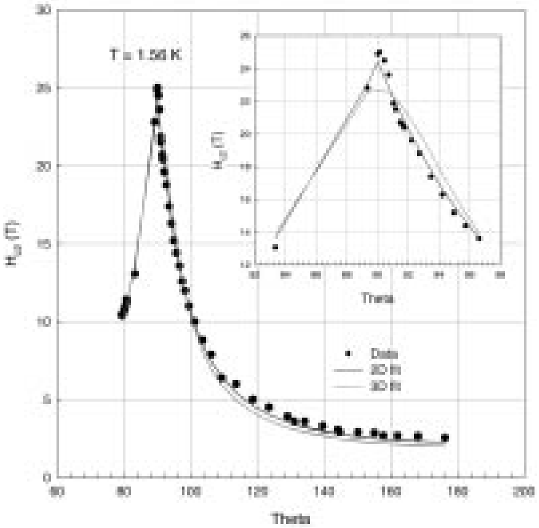

Figure 2. Angular dependence of the upper critical field. The solid lines are fits to 3D and 2D models. The inset is an expanded view near θ=90°.

The angular dependence is consistent with the high anisotropy of the title compound. For field parallel to the planes, the H_{c2} exceeds considerably the BCS Pauli limit. The linear temperature dependence and the large H_{c2} suggest unconventional superconductivity in these systems.

Reference:

1 Zuo. F., *et al*., to be published.